

relaxation times for both the conductivities are the same. This is perhaps a reasonable approximation when the electrons only are the main carriers for both heat and electricity. As a matter of fact the phonons also carry an appreciable portion of the thermal energy, specially at low temperatures, so that τ_{ph} and τ_e are not equal. The ratio $\frac{\tau_{ph}}{\tau_e}$ rather decreases at low temperatures, although the ratio may be of the order of unity at room temperature. The difference in τ_{ph} values for different materials gives rise to a difference in the value of L for different metals.

Measurements of the Fermi surface indicate that it is often non-spherical in shape. This contradicts the model, which predicts a spherical Fermi surface. This theory is incapable of explaining why some crystals have metallic properties while others are semiconductors and insulators.

The most important feature of this theory is that it destroys the notion of classical theory that all free electrons are conduction electrons. According to Sommerfeld's theory only few free electrons, whose energies lie in the vicinity of Fermi level, contribute to the mechanism of conduction and only those free electrons are called conduction electrons.

XXXVI. BAND THEORY OF SOLIDS

The quantum free electron theory of metals assumes that a conduction electron in a metal experiences a constant (zero) potential and so is completely free to move about in the crystal, restrained only by the surface of the crystal. This theory explains successfully the phenomena of specific heat, electrical

conductivity, thermionic emission, thermal conductivity and paramagnetism. Yet, there are many other physical properties which could not be explained by the free electron model. The model also failed to explain why some solids are good conductors of electricity, some are semiconductors and others are insulators.

When we considered the solid as a collection of free electrons in a box, we imposed the condition that the wave function vanishes at the walls of the box—that is, on the surface of the sample, allowing the conduction electrons to move in a region of constant potential. Obviously this approximation of the potential inside the crystal is too drastic.

It is now suggested to disregard the surface and to treat the crystal as an infinite array of lattice points. To do this, slightly different forms of boundary conditions, called cyclic or periodic boundary conditions, have been developed. Inside a real crystal, there is a periodic arrangement of positively charged ions through which the electrons move. The motion of a representative electron is shown in Fig. 6.42 (a). The potential of the electron at the positive ion site is zero and is maximum in between. So along any line passing through the centres of the positive ions, the potential variation must be as shown in Fig. 6.42 (b). We find that the potential varies periodically, with the same period as the lattice. We have now to study the motion of the electron in such a lattice and energy states it can occupy. The appropriate Schrödinger equation for the motion of the electron is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} [E - V(x)]\psi = 0 \quad (6.170)$$

where, the potential function $V(x)$ has the periodicity of the lattice given by

$$V(x) = V(x + a) \quad (6.171)$$

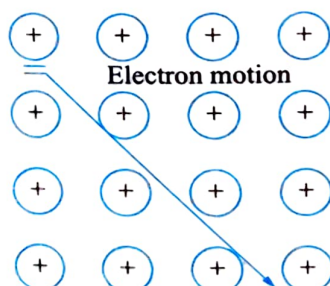
with a as the periodicity of the lattice.

Bloch has shown that an equation of the type (6.170) has a solution of the form

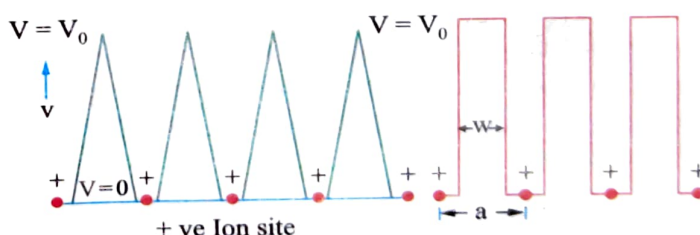
$$\psi(x) = u_K(x)e^{iKx} \quad (6.172)$$

where, $u_K(x)$ has the periodicity of the lattice given by

$$u_K(x) = u_K(x + a) \quad (6.173)$$



(a)



(b)

Fig. 6.42 One-dimensional periodic potential distribution for a crystal

K represents the state of the motion of the electron and K th state corresponds to an electron having a momentum, $p = \frac{hK}{2\pi}$ and a de Broglie wavelength λ is given by $\lambda = \frac{2\pi}{K}$. In the simple one-dimensional model we are considering, ' K ' is directed along the x -axis and, in the general case, K has to be treated as a vector, and so it is also called the propagation vector. The solution of equation (6.172) consists of a plane wave e^{iKx} modulated by the periodic function $u_K(x)$. With a sinusoidal type of potential inside as shown in Fig. 6.42 (b), the Schrödinger equation is not easily tractable. So Kronig and Penney introduced a simpler model for the shape of the potential variation. The potential inside the crystal is approximated to the shape of rectangular steps as shown in Fig. 6.43.

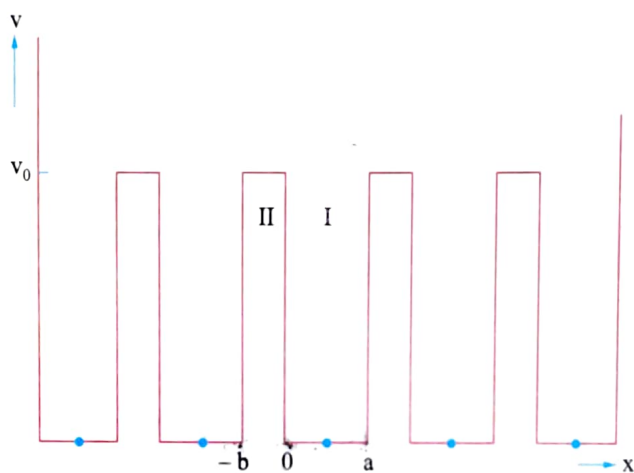


Fig. 6.43 Ideal periodic square well potential used by Kronig and Penney

XXXVII. ELECTRON IN A PERIODIC FIELD OF A CRYSTAL (THE KRONIG-PENNEY MODEL)

For the treatment of our problem, a periodic repetition of the potential well of Fig. 6.10, i.e., a periodic arrangement of potential wells and potential barriers, is most probably very close to reality and is also best suited for the calculation. Such a periodic potential is shown in Fig. 6.43 for the one-dimensional case.

Although this model is highly artificial, yet it illustrates many of the characteristic features of the behaviour of electrons in a periodic lattice. The wave functions associated with this model can be calculated by solving Schrödinger equations for the two regions I and II. The time-independent Schrödinger equation takes the following forms for the two regions

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} E\psi = 0; \text{ for } 0 < x < a \quad (6.173a)$$

and
$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E - V_0)\psi = 0; \text{ for } -b < x < 0 \quad (6.174)$$

Making use of Bloch's theorem, the solution can be written in the form

$$\psi(x) = u_K(x)e^{iKx} \quad (6.175)$$

Assuming that the total energy E of the electron is less than the potential energy V_0 , we define two real quantities α and β such that

$$\alpha^2 = \frac{8\pi^2 m E}{h^2} \quad (6.176)$$

$$\beta^2 = \frac{8\pi^2 m}{h^2} (V_0 - E) \quad (6.177)$$

Thus,

$$\frac{d^2 \psi}{dx^2} + \alpha^2 \psi = 0; \text{ for } 0 < x < a \quad (6.178)$$

$$\frac{d^2 \psi}{dx^2} - \beta^2 \psi = 0; \text{ for } -b < x < 0 \quad (6.179)$$

The solution that will be appropriate for both the regions suggested by Bloch is of the form

$$\psi(x) = u_K(x) e^{iKx}$$

On differentiating this equation, one gets

$$\frac{d\psi}{dx} = e^{iKx} \frac{du_K}{dx} + u_K iK e^{iKx}$$

$$\frac{d^2 \psi}{dx^2} = e^{iKx} \frac{d^2 u_K}{dx^2} + iK e^{iKx} \frac{du_K}{dx} + iK e^{iKx} \frac{du_K}{dx} - K^2 e^{iKx} u_K$$

$$\frac{d^2 \psi}{dx^2} = -K^2 e^{iKx} u_K + 2iK e^{iKx} \frac{du_K}{dx} + e^{iKx} \frac{d^2 u_K}{dx^2}$$

Substituting these values in equations (6.178) and (6.179), we get

$$\frac{d^2 u_1}{dx^2} + 2iK \frac{du_1}{dx} + (\alpha^2 - K^2) u_1 = 0; \text{ for } 0 < x < a \quad (6.180)$$

$$\frac{d^2 u_2}{dx^2} + 2iK \frac{du_2}{dx} - (\beta^2 + K^2) u_2 = 0; \text{ for } -b < x < 0 \quad (6.181)$$

where, u_1 represents the value of $u_K(x)$ in the interval $0 < x < a$ and u_2 the value of $u_K(x)$ in the interval $-b < x < 0$.

The solution of the differential equation (6.180) is of the form

$$u_1 = e^{mx}$$

$$\frac{du_1}{dx} = m e^{mx} \text{ and } \frac{d^2 u_1}{dx^2} = m^2 e^{mx}$$

Substituting these values in equation (6.180), we get

$$m^2 e^{mx} + 2iK m e^{mx} + (\alpha^2 - K^2) e^{mx} = 0$$

$$m^2 + 2iK m + (\alpha^2 - K^2) = 0$$

$$m = \frac{-2iK \pm \sqrt{-4K^2 - 4(\alpha^2 - K^2)}}{2}$$

$$m = -iK \pm i\alpha$$

i.e.,

$$m_1 = -iK + i\alpha = i(\alpha - K)$$

and

$$m_2 = -iK - i\alpha = -i(\alpha + K)$$

Thus, the general solution is

$$u_1 = A e^{m_1 x} + B e^{m_2 x}$$

$$u_1 = A e^{i(\alpha - K)x} + B e^{-i(\alpha + K)x}$$

(6.182)

where, A and B are constants.

Similarly equation (6.181) can be written as

$$m^2 + 2iKm - (\beta^2 + K^2) = 0$$

$$m = \frac{-2iK \pm \sqrt{-4K^2 + 4(\beta^2 + K^2)}}{2}$$

$$m = -iK \pm \beta$$

i.e.,

$$m_1 = -iK + \beta = (\beta - iK)$$

$$m_2 = -iK - \beta = -(\beta + iK)$$

Thus,

$$u_2 = C e^{m_1 x} + D e^{m_2 x}$$

$$u_2 = C e^{(\beta - iK)x} + D e^{-(\beta + iK)x}$$

(6.183)

where, C and D are constants. The values of the constants A , B , C and D can be obtained by applying the boundary conditions.

$$[u_1(x)]_{x=0} = [u_2(x)]_{x=0}; \left[\frac{du_1(x)}{dx} \right]_{x=0} = \left[\frac{du_2(x)}{dx} \right]_{x=0}$$

and

$$[u_1(x)]_{x=a} = [u_2(x)]_{x=-b}; \left[\frac{du_1(x)}{dx} \right]_{x=a} = \left[\frac{du_2(x)}{dx} \right]_{x=-b}$$

Applying these conditions, we get

$$(i) \quad (A + B) = (C + D)$$

(6.184)

$$(ii) \quad [A i(\alpha - K) e^{i(\alpha - K)x} - B i(\alpha + K) e^{-i(\alpha + K)x}]_{x=0} = [C(\beta - iK) e^{(\beta - iK)x} - D(\beta + iK) e^{-(\beta + iK)x}]_{x=0}$$

i.e.,

$$i(\alpha - K)A - i(\alpha + K)B = (\beta - iK)C - (\beta + iK)D$$

(6.185)

$$(iii) \quad A e^{i(\alpha - K)a} + B e^{-i(\alpha + K)a} = C e^{(\beta - iK)b} + D e^{-(\beta + iK)b}$$

(6.186)

$$(iv) \quad [A i e^{i(\alpha - K)x} (\alpha - K) - B i(\alpha + K) e^{-i(\alpha + K)x}]_{x=a} = [C(\beta - iK) e^{(\beta - iK)x} - D(\beta + iK) e^{-(\beta + iK)x}]_{x=-b}$$

$$i.e., \quad A i(\alpha - K) e^{i(\alpha - K)a} - B i(\alpha + K) e^{-i(\alpha + K)a}$$

$$= C(\beta - iK) e^{(\beta - iK)b} - D(\beta + iK) e^{-(\beta + iK)b}$$

(6.187)

Equations (6.184), (6.185), (6.186) and (6.187) will have non-vanishing solutions if and only if the determinant of the coefficients A , B , C and D vanishes. This requires that

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ i(\alpha - K) & -i(\alpha + K) & (\beta - iK) & -(\beta + iK) \\ e^{i(\alpha - K)a} & e^{-i(\alpha + K)a} & e^{-(\beta - iK)b} & e^{(\beta + iK)b} \\ i(\alpha - K) e^{i(\alpha - K)a} & -i(\alpha + K) e^{-i(\alpha + K)a} & (\beta - iK) e^{-b(\beta - iK)} & -(\beta + iK) e^{b(\beta + iK)} \end{vmatrix} = 0$$

N.B.: As the solution of the determinant is a separate mathematical work, equations (6.189) can be assumed, and the last part of band theory may be discussed accordingly.

Solution of the Determinant

(The details of the solution of the above is beyond of the scope of the students and hence the solution can be assumed.)

The above determinant can be written as

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ a & b & c & d \\ p & q & r & s \\ ap & bq & cr & ds \end{vmatrix} = 0$$

This is equal to

$$\begin{vmatrix} b & c & d \\ q & r & s \\ bq & cr & ds \end{vmatrix} - \begin{vmatrix} a & c & d \\ p & r & s \\ ap & cr & ds \end{vmatrix} + \begin{vmatrix} a & b & d \\ p & q & s \\ ap & bq & ds \end{vmatrix} - \begin{vmatrix} a & b & c \\ p & q & r \\ ap & bq & cr \end{vmatrix} = 0$$

$$\begin{aligned} \text{i.e.,} \quad & b(rds - crs) - c(qds - bqs) + d(qcr - rbq) - a(rds - crs) + c(pds - sap) - d(pcr - apr) \\ & + a(qds - bqs) - b(pds - aps) + d(pbq - apq) - a(qcr - bqr) \\ & + b(pcr - apr) - c(pbq - apq) = 0 \end{aligned}$$

Expanding

$$\begin{aligned} & brds - bcrs - cqds + cbqs + dqcr - drbq - ards + acrs + cpds - csap - dpcr + dapr \\ & + aqds - abqs - bpds + baps + dpbq - dapq - aqcr + abqr + bpcr - bapr \\ & - cpbq + capq = 0 \end{aligned}$$

In other words

$$\begin{aligned} & ab(ps + qr - qs - pr) + ac(sr + pq - qr + ps) + ad(pr + qs - rs - pq) + bc(qs + pr - sr - pq) \\ & + bd(rs + pq - rq - ps) + cd(qr + ps - qs - pr) = 0 \end{aligned}$$

$$\begin{aligned} \text{i.e.,} \quad & ab[q(r - s) - p(r - s)] + ac[q(p - r) - s(p - r)] + ad[r(p - s) - q(p - s)] + bc[p(r - q) - s(r - q)] \\ & + bd[p(q - s) - r(q - s)] + cd[q(r - s) - p(r - s)] = 0 \end{aligned}$$

$$\begin{aligned} \text{Thus} \quad & ab[(r - s)(q - p)] + ac[(p - r)(q - s)] + ad[(p - s)(r - q)] + bc[(r - q)(p - s)] \\ & + bd[(q - s)(p - r)] + cd[(r - s)(q - p)] = 0 \end{aligned}$$

$$\begin{aligned} \text{or} \quad & [(r - s)(q - p)][cd + ab] + (p - r)(q - s)[ac + bd] + (r - q)(p - s)[bc + ad] = 0 \\ \text{i.e.,} \quad & (p - r)(q - s)[bd + ac] + (r - q)(p - s)[bc + ad] = (s - r)(q - p)[ab + cd] \end{aligned}$$

Now substituting for a, b, c, d, p, q, r and s , we get

$$\begin{aligned}
 & [i(\alpha + K)(\beta + iK) + i(\alpha - K)(\beta - iK)] [e^{i(\alpha - K)a} - e^{-(\beta - iK)b}] [e^{-i(\alpha + K)a} - e^{(\beta + iK)b}] \\
 & + [-i(\alpha + K)(\beta - iK) - i(\alpha - K)(\beta + iK)] [e^{i(\alpha - K)a} - e^{(\beta + iK)b}] \\
 & [e^{-(\beta - iK)b} - e^{-i\alpha(\alpha + K)}] \\
 & = (\alpha^2 - K^2 - K^2 - \beta^2) [e^{-i\alpha(\alpha + K)} - e^{-i\alpha(\alpha - K)}] [e^{(\beta + iK)b} - e^{-b(\beta - iK)}] \\
 \text{i.e., } & (2i\alpha\beta - 2K^2) [e^{i(\alpha - K)a} - e^{-i(\beta - iK)b}] [e^{-i(\alpha + K)a} - e^{(\beta + iK)b}] + (-2i\alpha\beta - 2K^2) \\
 & [e^{i(\alpha - K)a} - e^{(\beta + iK)b}] [e^{-(\beta - iK)b} - e^{-i\alpha(\alpha + K)}] \\
 & = (\alpha^2 - \beta^2 - 2K^2) [e^{(\beta + iK)b} - e^{-b(\beta - iK)}] [e^{-i(\alpha + K)a} - e^{i\alpha(\alpha - K)}]
 \end{aligned}$$

R.H.S. is expanded as follows:

$$\begin{aligned}
 & = (\alpha^2 - \beta^2 - 2K^2) [e^{-i\alpha(\alpha + K)} e^{\beta b} e^{iKb} + e^{-i\alpha(K - \alpha)} e^{-\beta b} e^{-iKb} - e^{-i\alpha(\alpha + K)} e^{-\beta b} \\
 & e^{iKb} - e^{i\alpha\alpha} e^{\beta b} e^{iK(b - a)}]
 \end{aligned}$$

L.H.S. is now expanded as follows:

$$\begin{aligned}
 & (2i\alpha\beta - 2K^2) [e^{i\alpha(\alpha - K)} - i\alpha(\alpha + K) - e^{-b(\beta - iK)} - i\alpha(\alpha + K) + e^{-b(\beta - iK)} + b(\beta + iK) \\
 & - e^{i\alpha(\alpha - K)} + b(\beta + iK)] + (-2i\alpha\beta - 2K^2) [e^{-(\beta - iK)b} + i\alpha(\alpha - K) + e^{-i\alpha(\alpha + K)} + \\
 & b(\beta + iK) - e^{-i\alpha(\alpha + K)} + i\alpha(\alpha - K) - e^{b(\beta + iK)} - b(\beta + iK)]
 \end{aligned}$$

R.H.S. is further simplified as

$$\begin{aligned}
 & (\alpha^2 - \beta^2 - 2K^2) [e^{iK(b - a)} e^{\beta b} e^{-i\alpha a} + e^{iK(b - a)} e^{i\alpha a} e^{-\beta b} - e^{iK(b - a)} e^{-\beta b} e^{-i\alpha a} - e^{iK(b - a)} \\
 & e^{\beta b} e^{i\alpha a}]
 \end{aligned}$$

$$\text{R.H.S.} = (\alpha^2 - \beta^2 - 2K^2) (e^{iK(b - a)}) [e^{\beta b} (e^{-i\alpha a} - e^{i\alpha a}) + e^{-\beta b} (e^{i\alpha a} - e^{-i\alpha a})]$$

Simplifying L.H.S. further

$$\begin{aligned}
 & (2i\alpha\beta - 2K^2) [e^{-2i\alpha K} + e^{2i\alpha K} - e^{iK(b - a)} e^{-\beta b} e^{-i\alpha a} - e^{iK(b - a)} e^{i\alpha a} e^{\beta b}] \\
 & + (2i\alpha\beta - 2K^2) [e^{iK(b - a)} e^{-\beta b} e^{i\alpha a} + e^{iK(b - a)} e^{-i\alpha a} e^{\beta b} - e^{-2i\alpha K} - e^{2i\alpha K}]
 \end{aligned}$$

L.H.S. can be further simplified as

$$\begin{aligned}
 & (2i\alpha\beta - 2K^2) e^{iK(b - a)} [e^{-2i\alpha K} - iK(b - a) + e^{2i\alpha K} - iK(b - a) - e^{-\beta b - i\alpha a} - e^{i\alpha a + \beta b}] \\
 & + (2i\alpha\beta - 2K^2) e^{iK(b - a)} [e^{-\beta b} + i\alpha a + e^{\beta b} - i\alpha a - e^{-2i\alpha K} - iK(b - a) - e^{2i\alpha K} - iK(b - a)]
 \end{aligned}$$

Since $e^{iK(b - a)}$ is a common factor both for the L.H.S. and R.H.S., the equation is simplified and written as under: R.H.S.

$$\begin{aligned}
 & (\alpha^2 - \beta^2) [e^{\beta b} (e^{-i\alpha a} - e^{i\alpha a}) + e^{-\beta b} (e^{i\alpha a} - e^{-i\alpha a})] - 2K^2 [e^{\beta b} (e^{-i\alpha a} - e^{i\alpha a}) + e^{-\beta b} \\
 & (e^{i\alpha a} - e^{-i\alpha a})]
 \end{aligned}$$

L.H.S. is

$$\begin{aligned}
 & (2i\alpha\beta) [e^{-2i\alpha K} - iK(b - a) + e^{2i\alpha K} - iK(b - a) - e^{-\beta b - i\alpha a} - e^{i\alpha a + \beta b}] - 2K^2 [e^{-2i\alpha K} - iK(b - a) + e^{2i\alpha K} \\
 & - iK(b - a) - e^{i\alpha a + \beta b}] \\
 & (-2i\alpha\beta) [e^{-\beta b} + i\alpha a + e^{\beta b} - i\alpha a - e^{-2i\alpha K} - iK(b - a) - e^{2i\alpha K} - iK(b - a)] - 2K^2 [e^{-\beta b} + i\alpha a \\
 & + e^{\beta b} - i\alpha a - e^{-2i\alpha K} - iK(b - a) - e^{2i\alpha K} - iK(b - a)]
 \end{aligned}$$

On expanding K^2 terms of both L.H.S. and R.H.S. and equating them, we find the result yields zero value. Thus R.H.S. is equal to

$$(\alpha^2 - \beta^2) [-(e^{i\alpha a} - e^{-i\alpha a})e^{\beta b} + e^{-\beta a}(e^{i\alpha a} - e^{-i\alpha a})] = (\alpha^2 - \beta^2) [(e^{i\alpha a} - e^{-i\alpha a})(e^{\beta a} - e^{\beta a})]$$

$$= (\beta^2 - \alpha^2) [(e^{i\alpha a} - e^{-i\alpha a})(e^{\beta a} - e^{\beta a})]$$

L.H.S. is

$$2i\alpha\beta [2e^{-2i\alpha K - iK(b-a)} + 2e^{2i\beta K - iK(b-a)} - e^{-h\beta - i\alpha a} - e^{i\alpha a + h\beta} - e^{-h\beta + i\alpha a} - e^{h\beta - i\alpha a}]$$

$$= 2i\alpha\beta [2e^{-iK(a+b)} + 2e^{iK(a+b)}] - 2i\alpha\beta [e^{h\beta}(e^{i\alpha a} - e^{-i\alpha a}) + e^{-h\beta}(e^{i\alpha a} + e^{-i\alpha a})]$$

$$= 2i\alpha\beta [2e^{-iK(a+b)} + 2e^{iK(a+b)}] - 2i\alpha\beta [(e^{i\alpha a} + e^{-i\alpha a})(e^{h\beta} + e^{-h\beta})]$$

Now equating L.H.S. and R.H.S. and simplifying

$$\frac{(\beta^2 - \alpha^2)}{2i\alpha\beta} [(e^{i\alpha a} - e^{-i\alpha a})(e^{\beta a} - e^{\beta a})] = [2e^{-iK(a+b)} + 2e^{iK(a+b)}]$$

$$- [(e^{i\alpha a} + e^{-i\alpha a})(e^{h\beta} + e^{-h\beta})]$$

Dividing throughout by 2

$$\frac{(\beta^2 - \alpha^2)}{2\alpha\beta} \left[\frac{(e^{i\alpha a} - e^{-i\alpha a})}{2i} (e^{\beta a} - e^{-\beta a}) \right]$$

$$= [e^{iK(a+b)} + e^{-iK(a+b)}] - \left[(e^{i\alpha a} + e^{-i\alpha a}) \frac{(e^{h\beta} + e^{-h\beta})}{2} \right]$$

i.e.,

$$\frac{(\beta^2 - \alpha^2)}{2\alpha\beta} 2 \sin \alpha a \sin h \beta b = 2 \cos K(a+b) - 2 \cos \alpha a \cos h \beta b \quad (6.188)$$

(Thus the solution of the determinant (equation 6.187) is

$$\frac{(\beta^2 - \alpha^2)}{2\alpha\beta} \sin \alpha a \sin h \beta b + \cos h \beta b \cos \alpha a = \cos K(a+b) \quad (6.189)$$

Equation (6.189) is complicated but a simplification is possible. Kronig and Penney considered the possibility that $V_0 b$ remains finite. Such a function is called delta function. Under these circumstances, $\sin h \beta b \rightarrow \beta b$ and $\cos h \beta b \rightarrow 1$ as $b \rightarrow 0$. Hence equation (6.189) becomes

$$\frac{(\beta^2 - \alpha^2)}{2\alpha\beta} \beta b \sin \alpha a + \cos \alpha a = \cos Ka$$

Now,

$$(\beta^2 - \alpha^2) = \frac{8\pi^2 m}{h^2} (V_0 - E) - \frac{8\pi^2 m}{h^2} E = \left(\frac{8\pi^2 m}{h^2} \right) [V_0 - 2E]$$

Since $V_0 \gg E$,

$$\beta^2 - \alpha^2 = \frac{8\pi^2 m}{h^2} (V_0)$$

Substituting this in the above equation, we get

$$\left(\frac{8\pi^2 m V_0}{2\alpha \beta \hbar^2} \right) \beta b \sin \alpha a + \cos \alpha a = \cos Ka$$

where, $p = \frac{m V_0 ab}{\hbar^2}$

i.e.,

$$\left(\frac{m V_0 ab}{\hbar^2} \right) \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos Ka$$

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos Ka$$

(6.190)

The term $V_0 b$ is called the *barrier strength*. The term $P = \frac{m V_0 ab}{\hbar^2}$ in equation (6.190) is sometimes referred as the *scattering power* of the potential barrier. It is a measure of the strength with which electrons in a crystal are attracted to the ions on the crystal lattice sites. Also

$$\alpha^2 = \frac{8\pi^2 m E}{\hbar^2}, \text{ or } E = \frac{\alpha^2 \hbar^2}{8\pi^2 m}$$

and

$$K = \frac{2\pi}{\lambda} \quad (6.190a)$$

Equation (6.190) is a condition of the existence of a solution for the electron wave function.

There are only two variables in equation (6.190), namely α and K . The right hand side of equation (6.190) is bounded since it can only assume values between +1 and -1. If we plot the left-hand side of this equation against αa , it will be possible to determine those value of α (and hence energy) which are permissible; that is, permit $P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ to take values between +1 and -1.

When each of these values is set equal to $\cos Ka$, K is determined. Then α can be found from equation (6.180).

Figure 6.44 shows this plot for a value of P assumed arbitrarily as $3\pi/2$. Indicated in the figure are the permitted values of this function, shown as a solid line between white portions. This, then, gives rise to the concept of ranges of permitted values of α for a given ion lattice spacing a , and since

$E = \frac{\alpha^2 \hbar^2}{8\pi^2 m}$, permitted bands of energy are predicted. The following interesting conclusions may be drawn:

1. The allowed ranges of αa which permit a wave-mechanical solution to exist are shown by the shadow portions. Thus the motion of electrons in a periodic lattice is characterised by the bands of allowed energy separated by forbidden regions.

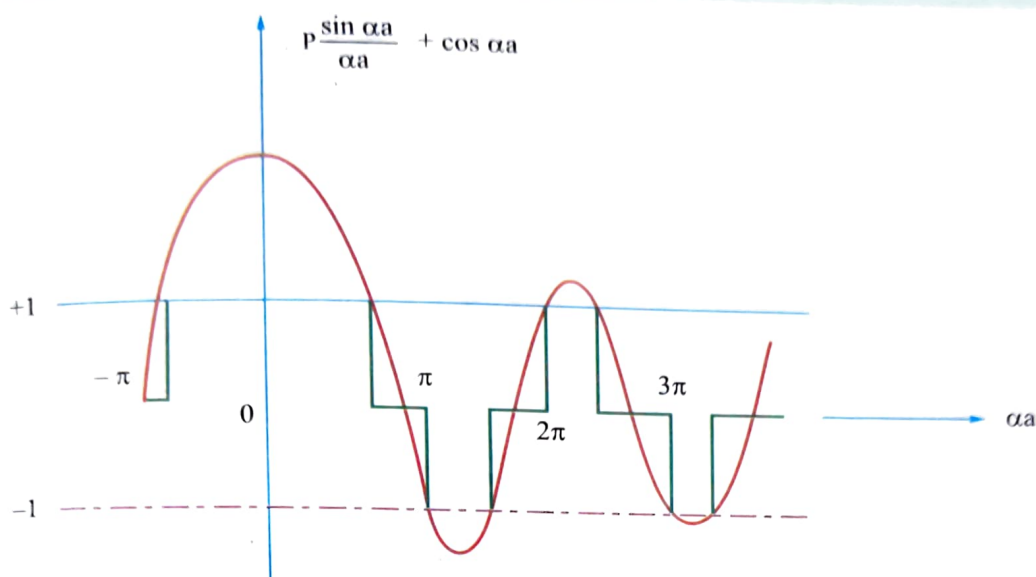


Fig. 6.44 Graph of $P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos Ka$ with $P = 3\pi/2$

- As the value of αa increases, the width of allowed energy bands also increases and the width of the forbidden bands decreases; this is a consequence of the fact that the first term of equation (6.190) decreases on the average with increasing αa .
- Let us now consider the effect of varying P . It is known that P is a measure of the potential barrier strength. If $V_0 b$ is a large, *i.e.*, if P is large, the function described by the left hand side of the equation (6.190) crosses $+1$ and -1 region at a steeper angle as shown in Fig. 6.45 (a). Thus the allowed bands are narrower and the forbidden bands are wider.

Also in equation (6.190), when $\alpha a = \pm n\pi$, $\cos \alpha a = \cos Ka$ with $Ka = \pm n\pi$; or $K = \pm \frac{n\pi}{a}$. These value of K are points of discontinuity in the $(E - K)$ curve for electrons in the crystal.

In the limit $P \rightarrow \infty$ the allowed band reduces to one single energy level; that is, we are back to the case of discrete energy spectrum existing in isolated atoms.

$P \rightarrow \infty$ it follows from equation (6.190) that $\sin \alpha a = 0$; or $\alpha a = \pm n\pi$

$$\alpha^2 = \frac{n^2 \pi^2}{a^2}$$

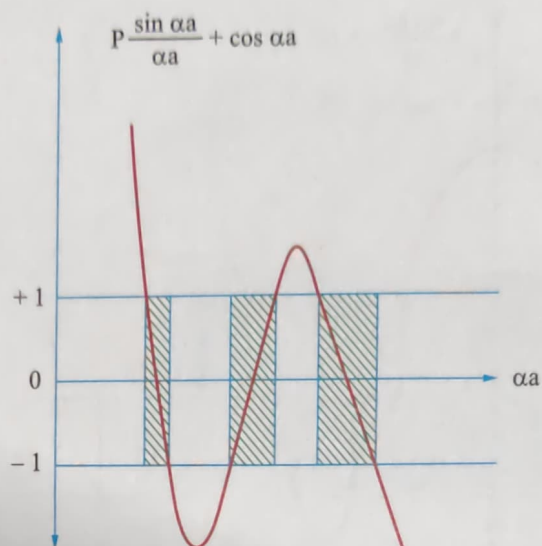
Referring equation (6.176),

$$\alpha^2 = \frac{n^2 \pi^2}{a^2} = \frac{2m E}{\hbar^2}$$

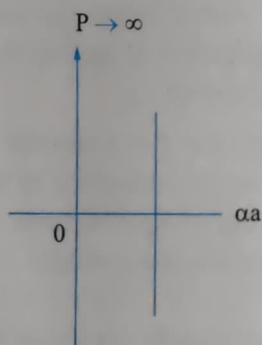
$$E = \left[\frac{n^2 \pi^2 \hbar^2}{a^2 2m} \right] = \left[\frac{n^2}{2ma^2} \right] \left[\frac{\pi^2 \hbar^2}{4\pi^2} \right]$$

$$E = \frac{n^2 \hbar^2}{8ma^2}$$

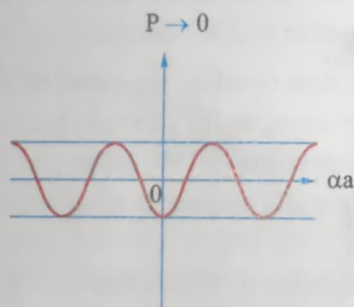
(6.191)



(a)



(b)



(c)

Fig. 6.45 (a) The left-hand side of equation (6.190) for $P = 3\pi/2$ as a function of αa ; (b) $P \rightarrow \infty$; (c) $P \rightarrow 0$

Here E is independent of K . The energy level in this case are discrete and the result is similar to the energy levels of a particle in a constant potential box of atomic dimensions. This is expected because for large P tunnelling through the barrier becomes almost improbable.

4. The other extreme case, when $P \rightarrow 0$, leads to

$$\cos \alpha a = \cos Ka$$

Thus,

$$\alpha = K$$

i.e.,

$$\alpha^2 = K^2$$

Referring equation (6.176),

$$K^2 = \alpha^2 = \frac{2m E}{h^2}$$

$$E = \left(\frac{h^2}{2m} \right) K^2$$

(6.191a)

$$E = \left(\frac{h^2}{8\pi^2 m} \right) \left(\frac{2\pi}{\lambda} \right)^2$$

Referring equation (6.190a)

$$E = \left(\frac{h^2}{2m} \right) \frac{1}{\lambda^2}$$

$$E = \left(\frac{h^2}{2m} \right) \frac{p^2}{h^2} = \frac{p^2}{2m} = \frac{1}{2} m v^2$$

(6.192)

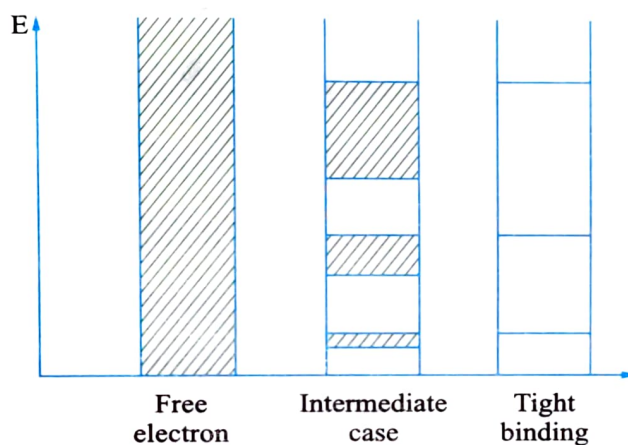


Fig. 6.46 Energy level structure for differentiating degrees of binding

Equation (6.192) is appropriate to completely free particles. Hence no energy levels exist; all energies are allowed to the electrons.

Thus by varying P from zero to infinity we cover the whole range, from the completely free electron to the completely bound electron.

XXXVIII. BRILLOUIN ZONES

The electron moving in a periodic potential lattice can have energy values only between allowed regions or zones. With the help of equation (6.109), it is possible to plot the total energy E of the electron versus the wave number, or the propagation vector ' K ', and the plot is shown in Fig. 6.47.

The right hand side of the equation (6.190) becomes ± 1 for values of $K = n\pi/a$, and hence the discontinuities in the E versus K graph occur at $K = n\pi/a$, where n takes the values of $\pm 1, \pm 2, \pm 3, \dots$ etc.